Description of Models
Applicable to Transport and Fate Thrust Area
CBNP Transport & Fate Team

CFD Models For Flow Around Buildings

- **Dynaflow**
- **FEM3C**
- **GASFLOW**
- **HIGRAD**
- **TEMPEST**

Mesoscale Atmospheric Models

- **COAMPS**
- **HOTMAC**
- **NORAPS**
- **RAMS**

Subway System & Interior Flow Models

- **GASFLOW**
- **SES**

Building Interior Flow and Transport Models

- **COMIS**
- **CONVEC9**
- **GASFLOW**
- **LBNL98**
- **LBNL Simple Duct Model**
- **MIAQ4**

Plume Dispersion Models

- **ADPIC**
- **HYPACT**
- **LODI**
- **RAPTAD**
- **SLAB**

Model Name	**Dynaflow**
Past Applications	This CFD code has been applied to flow and transport problems that involve arbitrarily complex geometry and require sufficiently fine-grid resolution and robust solution techniques. With some further development, the code could also be a highly useful tool for simulating local-scale atmospheric flows and the transport/diffusion of pollutants.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient and Steady State Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- 3 eqn. k-epsilon-A2 w/ non-linear anisotropic eddy viscosity (1.75 order)
Wall Shear Stress	No slip. Eqns. integrated to the wall.
Heat Transport	- solves temperature eqn.
Moisture Transport	- no moisture transport eqn.
Surface Heating	user-specified through B.C.'s
Dispersion	No internal dispersion modules. Flow fields can be used to drive Lagrangian dispersion models. Scalar advection/diffusion equation, but no source set-up
Chemistry	- No internal chemistry modules.
Numerics	- finite element - second-order projection method for time integration - modified forward Euler explicit scheme also available - 2nd order accurate in time and space - implicit pressure equation solved by direct solver or preconditioned conjugate gradient method - variables computed on staggered grid
Mesh	- unstructured grids (non-orthogonal) - variable grid spacing - irregular domains allowed - obstacles handled outside of computational domain

Dynaflow (cont.)

B.C.'s	specified in-flow, zero gradient, free-slip, no-slip, and specified flux
Input	- ascii input files; no graphical user interface
Output (Graphics)	- velocity and scalar fields are post-processed (plotting package used is GRIZ). Time history data can be post-processed by a X-Y plotting routine. - 3-d visualization by GRIZ - no run-time interface
Platforms	- Unix-based workstations and supercomputers (Cray Y-MP, DEC ALPHA , SGI) - vectorized version available
References model description:	Gresho, P.M. and S.T. Chan, 1990, "On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly consistent mass matrix, part 2: implementation," Int, J. for Num. Meth. in Fluids, 11:621-659. Christon, M.A., 1995, "HYDRA - A finite element computational fluid dynamics code: User's manual," UCRL-MA-121344, LLNL, Livermore, CA.
flow around obstacles:	Gresho, P.M. and S.T. Chan, 1997, "Projection 2 goes turbulent--and fully implicit," Int. J. Comp. Fluid Dyn. (in press).
evaluation studies:	Craft, T.J., B.E. Launder, and K. Suga, 1997, "Development and application of a cubic, non-linear eddy-viscosity model of turbulence," Int. J. Heat & FluidFlow (in press).
Comments	The code was developed mainly for solving engineering-type problems and thus some development is necessary in order to use it to simulate atmospheric flows and the transport/diffusion of pollutants. The current code derives from the Hydra CFD code.
Contact Person(s)	Stevens T. Chan, L-103 Atmospheric Science Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94551 Phone: (510) 422-1822 E-mail: schan@llnl.gov

Model Name	**FEM3C**
Past Applications	This CFD code has been applied to small-scale atmospheric flow and transport/diffusion of pollutants in which the effects of terrain and obstruction are important and/or the coupling between pollutants and flow field must be considered.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- Similarity-based K-theory (1st order) - 2 eqn. k-epsilon (1.5 order)
Wall Shear Stress	Traditional law-of-wall approach and specified turbulence stresses
Heat Transport	Solves temperature eqn.
Moisture Transport	No moisture transport.
Surface Heating	User-specified through B.C.'s
Dispersion	Eulerian dispersion algorithms are second-order accurate and used for solving the conservation equations of species - area and volume sources defined by grid cells. - multiple sources possible - dense or buoyant gas dispersion possible - phase change allowed (droplet/vapor) - no deposition or resuspension physics
Chemistry	- No internal chemistry modules.
Numerics	- finite element - explicit (modified forward Euler) - 2nd order accurate in time and space - pressure is determined by solving an implicit pressure equation (direct solver or pre-conditioned conjugate gradient method) - variables computed on staggered grid
Mesh	- structured grids (non-orthogonal) - variable grid spacing - irregular domains allowed - obstacles handled by "no flow" grids
B.C.'s	zero gradient, free-slip, no-slip, and specified flux

FEM3C (cont.)

Input	- ascii input files; no graphical user interface
Output (Graphics)	- Wind, concentration, and dosage fields for selected times are post-processed by a graphics code called GRIZ. Time history data of wind components and concentration for preselected locations are readily processed by a X-Y plotting routine. - 3-d visualization (GRIZ) - no run-time interface
Platforms	- Unix-based workstations and supercomputers (Cray Y-MP, DEC ALPHA , SGI) - vectorized version available
References model description:	Chan, S.T., 1994, "FEM3C-An improved three-dimensional heavy-gas dispersion model: User's manual," UCRL-MA-116567 Rev. 1, LLNL, Livermore, CA.
flow around obstacles:	Chan, S.T., 1992, "Numerical simulations of LNG vapor dispersion from a fenced storage area," Journal of Hazardous Materials, 30:195-224.
evaluation studies:	Ermak, D.L., S.T. Chan, D.L. Morgan, and L.K. Morris, 1982, "A comparison of dense gas dispersion model simulations with Burro series LNG spill test results," Journal of Hazardous Materials, 6:129-160. Chan, S.T., D.L. Ermak, and L.K. Morris, 1987, "FEM3 model simulations of selected Thorney Island phase I trials," Journal of Hazardous Materials, 16:267-292.
Comments	The FEM3C model has recently been used to simulate the dispersion of a line-source of trace gas (to simulate the release of C/B agents by terrorists from a moving truck) in the vicinity of the Capitol Building. Very plausible results have been obtained.
Contact Person(s)	Stevens T. Chan, L-103 Atmospheric Science Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94551 Phone: (510) 422-1822 E-mail: schan@llnl.gov

Model Name	**GASFLOW 2.0**
Past Applications	This CFD code has been used primarily to model flows inside facilities, between rooms, and around obstacles. Unique features include combustion and transport of flammable gases, chemical reactions, entrainment and deposition of aerosols, and heating/cooling of material surfaces.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Compressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Compressible or Incompressible - Newtonian - Sub or Supersonic - Laminar or Turbulent
Turbulence Scheme(s)	- Algebraic K-theory (1st order) - 2 eqn. k-epsilon (1.5 order)
Wall Shear Stress	- traditional law-of-wall approach, but modified with 1/7 power law - laminar sub-layer law-of-wall very close to sfc.
Heat Transport	- solves internal energy eqn.
Moisture Transport	- modeling through multiple species transport; condensation and vaporization on structures and droplet "rainout" possible; feedback through source or sink terms in mass and energy equations
Surface Heating	- 1d heat conduction through specified B.C.'s - no solar radiation, bldg. shadow, and surface radiation budget calculations
Dispersion	- Eulerian - through multiple gas species transport can have single or multi-grid source(s) - dense or buoyant gas dispersion possible - no deposition/resuspension - Lagrangian - discrete particle (aerosol) transport determined by fluid drag forces and Monte Carlo diffusion - deposition through particle bounce threshold velocity - entrainment through fluid drag/frictional force balance approach
Chemistry	- gaseous one-step global chemical kinetics (H2, NH3, CO, CH4 w/ O2 or NO2) with foundation for programming other reactions - no aerosol chemistry

GASFLOW 2.0 (cont.)

Numerics	- finite volume - implicit/explicit (ICEd-ALE scheme) - 1st order donor cell or 2nd order Van Leer advection schemes - Preconditioned Conjugate Residual method for solving Poisson pressure eqn. - variables computed on staggered grid
Mesh	- orthogonal mesh (rectangular & cylindrical) - variable (expanding) grid capability - rudimentary automatic mesh generation - obstacles defined by “no-flow” grid cells
B.C.’s	zero gradient, cyclic, pressure, velocity, slip, no-slip
Input	- ascii input file; no graphical user interface - no CAD interface
Output (Graphics)	- binary files for LANL-developed PSCAN (x-y, line contour, vector, grid mesh plots), plot types specified in input file - ascii column output for general plotting packages (e.g., Spyglass, XMGR, GMV) - no run-time interface
Platforms	- Unix-based workstations and supercomputers - vectorized form available, but no parallel version
References model description:	Lam et al., 1994, Hydrogen Mixing Studies User’s Manual, NUREG/CR-6180. Travis et al., 1994, GASFLOW: Theory and Computational Model, Vol. 1, LA-UR-94-2270.
flow around obstacles:	Lam et al., 1993, Hydrogen Mixing Studies Assessment Manual, NUREG/CR-6060.
evaluation studies:	Whicker, Yang, Rogers, and Spore, 1996, "Experimental characterization and computational modeling of indoor aerosol dispersion and their applications in optimization of continuous air monitor placement, " LA-UR-95-4174. Müller and Travis, 1994, "GASFLOW comparisons with Bureau of Mines Experiments," LA-UR-94-2020.
Comments	- DOE-DP recommended in-facility CFD code - NRC recommended containment (in-facility) CFD code - derives from LANL family of CFD codes (e.g., SOLA, KIVA) - includes combustion physics
Contact Person(s)	George Niederauer Los Alamos National Laboratory Group TSA-10, MS F575 Los Alamos, NM 87545 505-665-2538; georgen@lanl.gov

Model Name	**HIGRAD**
Past Applications	This CFD code has been used to generate potential flow over a sphere; resolve a flow field in the vicinity of buildings and/or steep hills; simulate small cumulus clouds; and resolve boundary-layer eddies over the Pacific warm pool.
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations (Transient Compressible or Incompressible Forms w/ buoyancy production))
Fluid Type and Flow Regimes	- Compressible or Incompressible - Newtonian - Sub or Supersonic - Laminar or Turbulent
Turbulence Scheme(s)	- Smagorinsky K-theory (1st order) - 1 eqn. k-l (1.5 order)
Wall Shear Stress	No current parameterizations are present in the code.
Heat Transport	Solves internal energy eqn.
Moisture Transport	A conservation equation for moisture transport is included and condensational effects are handled.
Surface Heating	- surface energy budget eqns., including both long and shortwave radiation, are currently being added; but no building shadow effects - no heat conduction through building materials
Dispersion	No internal dispersion modules. Flow fields can be used to drive Lagrangian dispersion models.
Chemistry	No internal chemistry modules.
Numerics	- finite volume - explicit - employs MPDATA advection scheme with monotone behavior or semi-Lagrangian scheme - second order accurate in time and space - pressure is diagnosed (compressible option) or is determined by solving an implicit pressure equation (pre-conditioned conjugate gradient method) (anelastic option)

HIGRAD (cont.)

Mesh	- nonorthogonal terrain following coordinate system (can easily incorporate orthogonal transformations) - numerics can handle expanding mesh - zero flow at obstacle grid points
B.C.'s	- side boundary conditions can either be cyclic, gradient equal to zero, or set to relax to specified environmental profiles - an absorbing layer can be activated at the top and either non-slip or free-slip boundary conditions can be imposed at the bottom.
Input	- ascii input file; no graphical user interface - input can include atmospheric sounding data and/or data interpolated from other models.
Output (Graphics)	- output has been fed into graphics packages such as AVS - no run-time interface
Platforms	- Unix-based workstations and supercomputers - Fortran 90 and Fortran 77 versions of the code exist - runs on both vector and parallel machines.
References model description: flow around obstacles: evaluation studies:	Smolarkiewicz, P.K., and L.G. Margolin, 1995: On forward-in-time differencing for fluids: An Eulerian/semi-Lagrangian nonhydrostatic model for stratified flows. LA-UR-94-4357.
Comments	
Contact Person(s)	Jon Reisner Los Alamos National Laboratory Group EES-8, MS D401 Los Alamos, NM 87545 505-665-1889; reisner@lanl.gov

Model Name	**TEMPEST**
Past Applications	This CFD code has been used primarily to model heating and cooling of reactor components and flows in complex terrain, around buildings, and inside residential structures. Unique features include .
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Boussinesq - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- 2 eqn. k-epsilon (1.5 order)
Wall Shear Stress	- traditional law-of-wall approach
Heat Transport	- solves potential temperature eqn.
Moisture Transport	no moisture transport eqns.
Surface Heating	- 1d heat conduction through specified B.C.'s - no solar radiation, bldg. shadow, and surface radiation budget calculations
Dispersion	- Eulerian - through single-species concentration eqn. (can have single or multi-grid source(s)) - dense or buoyant gas dispersion possible - no deposition/resuspension - Lagrangian - flow fields can be used to drive Lagrangian dispersion models.
Chemistry	- no internal chemistry modules.
Numerics	- finite volume - explicit for momentum eqns., implicit for other eqns. (SMAC scheme) - 1st order donor cell for advection - finite difference methods for solving Poisson pressure eqn. - variables computed on staggered grid
Mesh	- orthogonal mesh (rectangular & cylindrical) - expanding grid capability - rudimentary automatic mesh generation - obstacles defined by "no-flow" grid cells
B.C.'s	zero gradient, cyclic, velocity, slip, no-slip
Input	- ascii input file; no graphical user interface - no CAD interface

TEMPEST (cont.)

Output (Graphics)	- ascii output files for x-y, line contour, vector, grid mesh plots - no run-time interface
Platforms	- Unix-based workstations and supercomputers - vectorized form, but no parallel version
References model description:	Trent and Eyler, 1989, TEMPEST, A 3-d Time Dependent Computer Program for Hydrothermal Analysis, PNL-4348.
flow around obstacles:	Zhang, Arya, and Snyder, 1996, A comparison of numerical and physical modeling of stable atmospheric flow and dispersion around a cubical building, At. Env., v30, pp 1327-1345. Guenther, Lamb, and Stock, 1990, 3-d numerical simulation of plume downwash with a k-ε turbulence model, JAM, v 29, p 633.
Comments	Currently not actively used at PNNL.
Contact Person(s)	Pacific Northwest National Laboratory Richland, WA

Model Name	**COAMPS** (Coupled Ocean/Atmosphere Mesoscale Prediction System)
Applications	micro to mesoscale atmospheric weather forecasting (cloud scale to extratropical cyclone scale)
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations
Fluid Type and Flow Regimes	Fully compressible - Nonhydrostatic - Newtonian
Turbulence	TKE-epsilon (1.5 order) Large Eddy Simulation Capability
Wall Shear Stress	Vertical Mixing length at Earth's surface according to Mellor and Yamada (1974) or Therry and Lacarrere (1983)
Heat Transport	Solves Thermodynamic Energy Equation
Moisture	Explicit moist physics with Cumulus Parameterization
SurfaceTreatment	SurfaceLayerParameterization Heat and Moisture Transfer into the soil
Dispersion	None
Chemistry	None
Numerics	2nd order centered finite difference time splitting semi-Lagrangian in LES mode
Mesh	Staggered Grid (Arakawa-C grid) nesting capability for up to 7 grids
B.C.'s	From large scale weather prediction model or gridded analysis
Input	Namelist driven Binary (IEEE 32 bit standard) input/output
Output (Graphics)	NCARGRAPHICS post-processor Vis-5d capability
Platforms	Unix-based workstations and supercomputers (vectorized)
References	Hodur, R. 1997: Mo. Wea. Rev. in process Haack, T., 1996: Software User's Manual for the COAMPS , NRL
Comments	A state of the science operational and research model capable of simulating a broad spectrum of atmospheric circulation.
Contact Persons	Martin Leach Lawrence Livermore National Laboratory L-103 Livermore CA, 94550 510-422-5192; mleach@llnl.gov

Model Name	**HOTMAC**
Applications	Complex mesoscale flow in coastal, mountainous, and urban areas
Fluid Equations	Incompressible hydrostatic Navier-Stokes Equations
Fluid Type and Flow Regimes	Incompressible - Hydrostatic - Newtonian Terrain Following
Turbulence	2 equation q2-l closure (1.5 order) (similar to k-e) 1 equation q2 closure (1.5 order) (empirical equation for l)
Heat Transport	Solves potential energy equation
Moisture	Yes, condensation effects are also included Statistical description of clouds based on moisture content.
SurfaceTreatment	Surface heating: long and shortwave radiation, sensible, latent, and soil heat flux are accounted for with 13 different land classes available. Urban canopy: model has parameterizations for canopy-induced momentum drag, turbulent kinetic energy production, and longwave/shortwave attenuation, as well as urban landclass properties.
Dispersion	RAPTAD model
Chemistry	None
Numerics	ADI (alternating direction implicit) numerical algorithm. Relatively fast compared to most numerical schemes since it allows for a 1 to 10 minute timestep.
Mesh	Rectilinear terrain following coordinate system wiht expanding mesh in the vertical direction (typically use Dz = 2 m near surface) and nested grids in the horizontal (typically Dx=1, 3, 9 km or 2, 6, 18 km)
B.C.'s	I.C's: Typically use rawinsonde for vertical profiles of T, ws, wd, rh, and assume horizontal homogenity. Need 6-12 hour spin-up time to overcome initialization approximations. Also have the capability to use mutiple vertical profiles. Nudging: Uses simple 4-d data assimilation scheme for winds. Can use single or multiple vertical profiles and define a horizontal cone of influence.
Input	ASCII file
Output (Graphics)	Formats for NCAR graphics, Spyglass 2D & 3D software, AVS & Deltagraph.
Platforms	Fortran77 version of the code exist for Unix and IBM platforms
References	Model description: Yamada and Bunker, 1989: A Numerical Model study of Nocturnal Drainage Flows with Strong Wind and Temperature Gradients, *JAM, 28*, pp 545-554 Urban Canopy - Brown and Williams, 1997: the Effect of Urban Canopy Parameterizations on Mesoscale Meteorological Model Simulations in the Paso del Norte Area, 90th AWMA Conf., Toronto, Canada.
Contact Persons	Mike Williams or Michael Brown Energy & Environmental Analysis Group Los Alamos National Laboratory Los Alamos, NM 87545 (505) 667-1788

Model Name	**NORAPS** (Navy Operational Regional Atmospheric Prediction System**)**
Applications	regional atmospheric weather forecasting
Fluid Equations	Reynolds-Averaged Hydrostatic Primitive Equations in s coordinates
Fluid Type and Flow Regimes	Fully compressible - hydrostatic - Newtonian
Turbulence	TKE-epsilon (1.5 order)
Wall Shear Stress	
Heat Transport	Solves Thermodynamic Energy Equation
Moisture	Nonconvective precipitation occurs when supersaturation occurs at a grid point. Cumulus Parameterization of Kuo
SurfaceTreatment	SurfaceLayerParameterizationofDeardorff Ground temperature calculated from surface energy budget of Blackadar
Dispersion	None
Chemistry	None
Numerics	Split-explicit time integration scheme of Madala
Mesh	Staggered Grid (Arakawa-C grid) nesting capability for up to 3 grids
B.C.'s	From large scale weather prediction model or gridded analysis
Input	Namelist driven Binary (IEEE 32 bit standard) input/output
Output (Graphics)	NCARGRAPHICS post-processor Vis-5d capability
Platforms	Unix-based workstations and supercomputers (vectorized and parallel)
References	Hodur, R.M., 1982: Description and evaluation of NORAPS: The Navy operational regional atmospheric prediction system. *Mon. Wea. Rev.*, **100**, pp 1591-1602. Hodur, R.M., 1987: Evaluation of a regional Model with an update cycle. *Mon. Wea. Rev.*, **115**, pp 2707-2718.
Comments	Has been running operationally at the Fleet Numerical Meteorological and Oceanagraphic Center for a number of years.
Contact Persons	Martin Leach Lawrence Livermore National Laboratory L-103 Livermore CA, 94550 510-422-5192; mleach@llnl.gov

Model Name	**RAMS** (Regional Atmospheric Modeling System)	
Applications	micro to mesoscale atmospheric weather forecasting (cloud scale to extratropical cyclonescale)	
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations	
Fluid Type and Flow Regimes	Fully compressible - Nonhydrostatic - Newtonian Terrain Following	
Turbulence	First Order K theory, 1.5 order TKE Deardorff for large eddy simulations	
Wall Shear Stress	Louis (1979) surface layer parameterization vertical mixing Mellor and Yamada (1981)	
Heat Transport	Solves thermodynamic energy equation	
Moisture	Bulk microphysics for 7 condensate species cumulus parameterization	
SurfaceTreatment	Prognostic surface energy balance Vegetation, heat and moisture into soil	
Dispersion	HYPACT model	
Chemistry	None	
Numerics	Second or sixth order centered finite difference Hybrid forward scheme Leapfrog momentum Time splitting	
Mesh	Staggered grid (Arakawa-C grid) Nesting capability for n grids	
B.C.'s	From large scale weather prediction model or gridded analysis and single sounding	
Input	Namelist driven Binary (IEEE 32 bit standard) input/output	
Output (Graphics)	NCAR GRAPHICS post-processor AVS capability	
Platforms	Unix-based workstations and supercomputers vectorized and parallelized	
References	Many but Pielke et al. (1992) is most general	
Comments	A state of the science operational and research model capable of simulating a broad spectrum of atmospheric phenomena	
Contact Persons	James E. Bossert Los Alamos National Laboratory Mail Stop D-401 Los Alamos, NM 87545 (505) 667-6268	Craig Tremback ASTER division Mission Research Corporation Box 466 Fort Collins, CO 80526 (970) 282-4400

Name:	**Subway Environmental Simulation (SES) Model**
Past Applications	-Used in design of subway lines in following subway systems: Atlanta, Baltimore, Boston, Buffalo, Caracas, Chicago, Dallas, Hong Kong, Los Angeles, Minneapolis, Montreal, New York City, Philadelphia, Pittsburgh, San Francisco, Singapore, Taipei, and Washington DC.
Predictive Capability	-Predicts time-dependent history of temperature, humidity, and air velocity throughout entire subway system including tunnel, station, and ventilation shafts including effects of moving trains.
Model Approach	-one-dimensional. -based on conservation equations of mechanical energy, mass, and heat energy applied to individual control volumes representing segments of subway system. -control volume relationships form a set of linear ordinary differential equation that are solved as function of time.
Key Model Features: 1. Train Performance	Predicts: -total heat released by trains, passengers, and ancillary equipment such as air conditioning as function of time for entire system. -location of each train in system as function of time including acceleration and braking. -power demand, line current, and energy consumption (including tractive effort for each train and segment) for each train as function of time.
2. Aerodynamic Effects	-predicts time-dependent aerodynamic drag acting on each train in the system as function of specific train location and speed. -pressure changes caused by trains, fans, and buoyancy in vent shafts; viscous and minor losses computed.
3. Temperature/Humidity Effects including Heat Sink Effects	Accounts for: -localized heat/humidity sources and sinks (including train and station heat loads). -long-term heat conduction between subway and surrounding earth. -passenger sensible and latent heat included in analysis.
Dispersion	-No algorithm for dispersion of pollutants, but ANL has developed algorithm to predict dispersion using SES-predicted air flows. -Fire effects algorithm in SES predicts adequacy of emergency ventilation including buoyancy in tunnels, throttling at fire site, wall temperature, radiation effects, and modified viscous losses.
Chemistry	-No chemistry of pollutants accounted for at this time.
Mesh	-Entire subway system divided into line segments, each with cross-sectional areas and perimeters. -Subway alignment includes multiple track areas, junctions, portals, and nodal points. -Fan and ventilation shaft locations, lengths, cross-sectional areas, and perimeters used along with dimensions of dampers and gratings.
Input	-Graphical user interface to be available from U.S. DOT in March 1997. -Otherwise input is manual and includes general system data, train performance data, aerodynamic data, and temperature/humidity data.
Output	-Detailed printout of all dynamic parameters at specific time intervals is made to file and hard copy. -Time-dependent variables available. -No plots or visualization available at this time.
Platforms	-Runs on PC in real time.

References	-1. Subway Environmental Design Handbook (1980), Volume I. Principles and Application, 2nd Edition; Volume II. Subway Environmental Simulation (SES) Computer Program, Volume II, Part 1: User's Manual; and Volume II. Subway Environmental Simulation (SES) Programmer's Manual, U.S. Department of Transportation, 1980.
Comments	-Used throughout world for new subway design and emergency ventilation design and planning. -Code is in public domain since it was funded by U.S. DOT and city transit authorities. -Recommended by U.S. DOT for subway system flow and smoke studies.
Contact Person	-At DOE labs, contact is: Tony Policastro EAD/Building 900 Argonne National Laboratory 9700 South Cass Avenue Argonne, Illinois 60439 630-252-3235; policastro@anl.gov

1	Name	**COMIS** (Conjunction of Multizone Infiltration Specialists)
2	References	Feustel, H. E.: Annex 23 - An International Effort in Multizone Air Flow Modeling, In: *Proceedings, ROOMVENT '96*, July 1996, Yokohama H.E. Feustel, A. Raynor-Hooson (Editors): COMIS Fundamentals, Air Infiltration and Ventilation Centre, Technical Note 29, Lawrence Berkeley Laboratory Report, LBL-28560, 1990 Feustel, H.E., F. Allard, V.B. Dorer, M. Grosso, M. Herrlin, M. Liu, J.C. Phaff, Y. Utsumi, and H. Yoshino: The COMIS Infiltration Model, In: *Proceedings, Building Simulation '89*, The International Building Performance Simulation Association, Vancouver, 1989 Dorer, V. and A. Weber: Output Options for COMIS, Internal Annex Report, EMPA Dübendorf, 1995 Fürbringer, J.M., C.-A. Roulet, and R. Borchiellini: Annex 23 Subtask II&III Report - Evaluation of COMIS, Vol. 1 and Vol. 2, EPFL Lausanne, Switzerland, 1996
3	Abstract	COMIS is a multizone air flow and transport model. In terms of air-mass flow, buildings represent complicated interlacing systems of flow paths. In this grid-system the joints represent the zones of the building and the connections between the joints simulate the air flow paths. These include the flow resistances caused by open or closed doors and windows and air leakage through the walls. The boundary conditions for the pressure are described by grid points outside the building. Because of the nonlinear dependency of the flow rate on the pressure difference, the pressure distribution for a building can be calculated only by using a method of iterations.
4	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program Building 90, Room 3074 Berkeley, CA 94720, USA
5.	Information Contacts	Helmut E. Feustel Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program Building 90, Room 3074 Berkeley, CA 94720, USA
6	Application	Air flow distribution and pollutant transport mechanismn in single-zone and multizone buildings.
7	Limitations	Availability of flow characteristics of zone envelopes and outside pressure distribution and outdoor concentration data. Zones are defined as fully mixed volumes with a constant concentration level of the enclosed gas mixture representing a uniform pressure.
8	Sponsors	Department of Energy, International Energy Agency
9	Computer Requirement	FORTRAN 77 source code runs on all computer platforms if FORTRAN compiler is available.

10	Source-Receptor Relationship	Sources can be specified anywhere on a three-dimensional grid. Zones are handled as fully mixed.
11	Emission Rate	Each zone can have one source/sink for up to five airborne contaminants.
12	Chemical Composition	N/A
13	Plume Behavior	N/A
14	Wind Field	Complicated wind pressure distributions have to be provided by the user.
15.	Dispersion Algorithms	N/A
16	Chemical Reactions	N/A
17	Removal Process	Sink terms can be specified for each zone
18	Boundary conditions	Pressure field around the building, temperature field, outdoor concentrations
19	Meteorological Requirements	Wind speed at reference height for pressure coefficients, outdoor temperature, outdoor humidity, barometric pressure.
20	Evaluation	Model has successfully been evaluated by the Energy Conversation in Buildings and Community Systems implementing agreement. Analytical evaluation, inter-model comparison, user-tests, and comparison with in-situ experiments were performed.
21	Output	COMIS output include all interzonal air flows, nodal pressures, driving pressures for air flows, distribution of concentrations
22	Genealogy	COMIS was initially developed by the COMIS Workshop. Evaluation and further development took place in the frame of IEA ECBCS's Annex 23. COMIS now has the following features: Several air flow components, including cracks, large vertical openings, ducts, passive stacks, fans, flow controllers. Variable time step for air flow modeling, fixed time step based on time constant of critical zone for pollutant concentrations. Zone layers Schedules for leakage distribution, fan operation, and source/sink terms. Calculation of pressure coefficients for simple buildings.
23	Availability	see 5.

1.	Model Name	**CONVEC9**
2.	References :	Bauman, F., A. Gadgil, R. Kammerud, E. Altmayer, and M. Nansteel. (1983) Convective heat transfer in buildings: Recent research results. *ASHRAE Transactions*, **89**:1A, 215-233. Gadgil, A.; Bauman, F.; Altmayer, E.; Kammerud, R.C. (1984) Verification of a numerical simulation technique for natural convection. *Tansactions of the ASME. Journal of Solar Energy Engineering*, **106**, (no.3): 366-9. Gadgil, A.. and D. Gobin. (1984) Analysis of two-dimensional melting in rectangular enclosures in presence of convection. *Transactions of the ASME. Journal of Heat Transfer*, **106**, (no.1): 20-6. Nazaroff, W.W., D. Dong, and A. J. Gadgil. (1992) Numerical Investigations of the Deposition of Unattached 218PO and 212PB from Natural Convection Enclosure Flow, *Journal of Aerosol Sciences*, **23(4)**: 339-352.
3.	Abstract	Series of CFD codes developed and used to model natural and forced convection, for internal and external flows, in two and three dimensions, for complex interiors of rooms (e.g., internal partitions, furniture); includes heat and pollutant sources and sinks, and velocity sources and sinks (e.g., fans, windows). Simulation of laminar and turbulent flows for typical building conditions.
4.	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program,Building 90, Room 3058 Berkeley, CA 94720, USA
5.	Contact Person(s)	Ashok Gadgil Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program; Building 90, Room 3074 Berkeley, CA 94720, USA
6.	Applications	Heat transport and air flow in a room; accurate calculation of heat transfer coefficients; deposition of radon progeny on interior surfaces of an enclosure; investigation of ozone deposition on interior surfaces of a room.
7.	Limitations	Research model. No user's manual. No user-friendly input/output interfaces. Limited to rectilinear details on walls and partitions.
8.	Sponsors	U.S. Dept. Energy
9.	Computer Requirements	Developed for single processor machines. Code language is FORTRAN
10.	Conservation equations	Energy and mass transport and conservation. Arbitrary sources and sinks of fluid mass and heat in the space and on the bounding surfaces can be modeled
11.	Emissions rates	User-specified emission rates for surfaces and inside space
12.	Fluid Equations	3 Dimensional Navier Stokes Solver
13.	Fluid properties	Building air modeled as an incompressible Boussinesque fluid
14.	Turbulence Scheme(s)	Two equation turbulence models (k-epsilon / k-omega) modified for low Reynolds number turbulence
15.	Heat Transport	Transport by convection only, no radiation model
16.	Dispersion	- dense or buoyant gas dispersion possible - deposition modeled in detail
17.	Chemistry	Not available

18.	Numerics	Based on Patankar-Spalding differencing using the SIMPLE and SIMPLER algorithms developed at Imperial College and University of Minnesota; Alternating Direction Implicit solver
19.	Mesh	Non-uniform rectilinear Cartesian grids, staggered for velocity and pressure solutions. Can easily incorporate blockages and "frozen off" solid sections in the fluid space
20.	Boundary conditions	Periodic, pressure, pressure-gradient, velocity, slip, no slip
21.	Input	ASCII input file No user friendly graphical interface
22.	Output (Graphics)	ASCII column output for general plotting packages but no conversion codes; no run-time interface
23.	Evaluations	CONVEC2 model predictions and measurements of local Nusselt numbers compared

1.	Model Name	**GASFLOW 2.0**
2.	References Model description: Flow around obstacles: Evaluation studies:	Lam et al., 1994, Hydrogen Mixing Studies User's Manual, NUREG/CR-6180. Travis et al., 1994, GASFLOW: Theory and Computational Model, Vol. 1, LA-UR-94-2270. Lam et al., 1993, Hydrogen Mixing Studies Assessment Manual, NUREG/CR-6060. Lam et al., 1993, Hydrogen Mixing Studies Assessment Manual, NUREG/CR-6060. Breitung, W., P. Royl, J.R. Travis, and H. Wilkening. (1996) Analyses of hydrogen dispersion - GASFLOW computer program for determination of hydrogen distribution in pressurized water reactors. *ATW-International Zeitschrift fur Kernergie*, **41** (N6):411-416. J. P. Royl, J. R. Travis, E. A. Haytcher, and H. Wilkening, "Analysis of Mitigating Measures during Steam/Hydrogen distributions in Nuclear Reactor Containments with the 3D Field Code GASFLOW," presented at the OECD/NEA CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques, Winnipeg, Canada, May 13–15, 1996. K. Whicker, Y. Yang, J. Rogers, and J. Spore, "Experimental characterization and computational modeling of indoor aerosol dispersion and their applications in optimization of continuous air monitor placement, " LA-UR-95-4174, presented at the ASME Fluids Engineering Division Summer Meeting, July 1996. L. P. Royl, C. Müller, J. R. Travis, T. Wilson, "Validation of GASFLOW for Analysis of Steam/Hydrogen Transport and Combustion Processes in Nuclear Reactor Containments," Procs 13th Conference on Structural Mechanics in Reactor Technology, August 13-18, 1995 Porto Alegre, RS, Brazil C. Müller and J. R. Travis, "GASFLOW comparisons with Bureau of Mines Experiments," LA-UR-94-2020, presented at the American Nuclear Society 1994 Winter Annual Meeting, November 13-17, 1994.
3.	Abstract	This CFD code has been developed and used primarily to model flows inside geometrically complex nuclear containment facilities and around obstacles, such as walls, cabinets and other structures. Unique features include combustion and transport of flammable gases, chemical reactions, entrainment and deposition of aerosols, and heating/cooling of material surfaces.
4.	Location	Los Alamos National Laboratory Group TSA-10, MS F575 Los Alamos, NM 87545
5.	Contact Person(s)	GeorgeNiederauer Los Alamos National Laboratory, Group TSA-10, MS F575 Los Alamos, NM 87545 505-665-2538; georgen@lanl.gov
6.	Applications	Applicable to containment buildings, tanks, single rooms with and without ventilation systems. Applicable to multi-species gas mixing and transport problems, as well as aerosol transport problems
7.	Limitations	Major assumptions include: each cell is well mixed, each gas species has the same velocity at cell boundaries; agglomeration is currently ignored in the aerosol model; diffusion of species is based on mixture diffusion equations; gases assumed to behave as ideal gases; choking is currently not considered in the ventilation system components.

8.	Sponsors	LANL, U.S. Department of Energy; Nuclear Regulatory Commission
9.	Computer Requirements	- Unix-based workstations and supercomputers - Vectorized form available, but no parallel version
10.	Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Compressible Form w/ buoyancy production)
11.	Fluid Type and Flow Regimes	- Compressible or Incompressible - Newtonian - Sub or Supersonic - Laminar or Turbulent
12.	Turbulence Scheme(s)	- Algebraic K-theory (1st order) - 2 eqn. k-epsilon (1.5 order)
13.	Wall Shear Stress	- traditional law-of-wall approach, but modified with 1/7 power law - laminar sub-layer law-of-wall very close to sfc.
14.	Heat Transport	- solves internal energy equation
15.	Moisture Transport	Modeling of flow through multiple species transport and of condensation and vaporization on structures and droplet "rainout", with feedback through source or sink terms in mass and energy equations
16.	SurfaceHeating	- 1d heat conduction through specified boundary conditions - hardwired radiation heat transfer model for simple geometries can easily be added easily by Fortran programming
17.	Dispersion	Eulerian: - through multiple gas species transport can have single or multi-grid source(s) - dense or buoyant gas dispersion possible - no deposition/resuspension Lagrangian: - discrete particle (aerosol) transport determined by fluid drag forces and Monte Carlo diffusion - deposition/resuspension through particle bounce threshold velocity - entrainment through fluid drag/frictional force balance approach
18.	Chemistry	- gaseous: one-step global chemical kinetics (H_2, NH_3, CO, CH_4 w/ O_2 or NO_2); foundation for programming other chemical kinetics - no aerosol chemistry
19.	Numerics	Finite volume; implicit/explicit (ICEd-ALE scheme); 1st order donor cell or 2nd order Van Leer advection schemes; Preconditioned Conjugate Residual method for solving Poisson pressure eqn.; variables computed on staggered grid
20.	Mesh	Orthogonal mesh (rectangular & cylindrical); variable grid size capability; rudimentary automatic mesh generation; obstacles defined by “no-flow” grid cells
21.	Boundary conditions	- zero gradient, cyclic, pressure, velocity, slip, no-slip
22.	Input	- ascii input file; initial graphical user interface coming in summer 1997 - no CAD interface (planned for FY98)
23.	Output (Graphics)	- binary files for LANL-developed PSCAN (x-y, line contour, vector, grid mesh plots), plot types specified in input file; ascii column output for general plotting packages (e.g., XMGR, Spyglass), but no conversion codes; no run-time interface - initial graphical user interface coming in summer 1997
24.	Evaluations	Validated against data from many international experiments, from benchtop tests to 10-story high facilities using mixtures of different gas species and aerosols in a wide variety of conditions from quiescent to highly turbulent conditions
25.	Comments	- DOE-DP recommended in-facility CFD code - NRC recommended containment (in-facility) CFD code - derives from LANL family of CFD codes (e.g., SOLA, K-FIX, KIVA) - includes combustion physics

1	Name	**MIAQ4**
2	Reference	Nazaroff, W. W. and G. R. Cass. (1989) Mathematical Modeling of Indoor Aerosol Dynamics, *Environmental Science and Technology*, **23**: 157-166.
3	Abstract	MIAQ4 is a model of aerosol behavior within interior spaces, accounting for the effects of ventilation, filtration, deposition, coagulation and direct emission. It permits the tracking of the aerosol concentration and size distribution as a function of time, along with the accumulation of deposited materials on surfaces with various orientations. The model has been evaluated with data from experiments using environmental tobacco smoke and reasonable agreement was obtained.
4	Location	LBNL and UC Berkeley
5	Information Contact	Richard Sextro, LBNL William Nazaroff, UC Berkeley (and LBNL)
6	Application	Indoor aerosol behavior, permitting estimates of inhalation exposures to aerosols as a function of size and the accumulation of materials on surfaces as a secondary source of exposure
7	Limitations	The model treats indoor aerosol concentrations as being spatially uniform (well-mixed) and thus does not account for aerosol dispersion from sources. Interior airflow conditions are not treated as a continuum, but are assumed to fall into three different regimes.
8	Sponsors	Original work done as part of Nazaroff Ph.D. dissertation at Caltech (Nazaroff and Cass 1989); current and recent uses funded by a variety of sponsors, including U.S. DOE.
9	Computer requirement	Source code is in FORTRAN; will run on workstation or fast PC platforms
10	Source-receptor relationship	The model can treat multiple rooms, specifying air flow between the rooms as the transport process, along with the filtration efficiency for filters incorporated in an HVAC system. Sources may be located within any of the rooms, subject to the previously noted assumption that the interior concentrations are well mixed.
11	Emission rate	Emissions are treated as constant per unit time, with specification of the appropriate start and stop time, or as time varying, done as discrete steps each with a constant source rate for a given time period.
12	Chemical composition	The model currently treats the aerosols as spheres of uniform composition and assumes that the interaction between the aerosols and the surfaces (including other aerosols) is physical (and inelastic).
13	Plume behavior	N/A
14	Wind Field	Interior air flows along surfaces are treated as either 1) natural convection, 2) homogeneous turbulence or 3) forced laminar flow parallel to the surface of interest.
15	Dispersion Algorithms	N/A
16	Chemical reactions	The current model version does not explicitly account for chemical behavior but such a module could easily be added to the present model
17	Removal processes	As noted, the interaction with surfaces is assumed to take the form of inelastic collisions (if surface chemical effects can be specified, this interaction could be incorporated into the model. Coagulation, ventilation and surface deposition are accounted for. Surface deposition depends upon surface orientation and their thermal condition with respect to the room interior.
18	Boundary conditions	Dimensions of surfaces; initial conditions include specification of starting aerosol size distribution and concentration (if any) for indoors or for outdoors when infiltration is included in the problem

19	Meteorological requirements	Interior air and surface temperatures (or alternatively temperature differences)
20	Evaluation	MIAQ4 has been validated against ETS data (Nazaroff and Cass 1989).
21	Output	Tabular outputs (flat ASCII files) which can be ported to various graphics programs to provide time series plots, 2-D concentration plots, etc.
22	Genealogy	See 8 above. MIAQ4 has been used to examine the behavior of aerosols indoors, from estimating exposures to environmental tobacco smoke (Miller-Leiden *et al.* 1993) and evaluating engineering controls for ETS (Miller-Leiden and Nazaroff 1996) to the soiling of museum artwork by deposition of indoor aerosols (Nazaroff *et al.* 1990).
23	Availability	See 5 above.

1	Name	**LBNL simple duct model**
2	Reference	Carrie, F. R. and M. P. Modera. Particle Deposition in a Two-Dimensional Slot from a Transverse Stream, *Aerosol Science and Technology* (Submitted); LBL Report LBL-34829 (1995)
3	Abstract	The LBNL simple duct model is based on a set of analytical expressions for different air flow regimes, treating the problem in steady-state. It computes the deposition losses in - or alternatively the penetration through - ducts as a function of aerosol size and density, duct dimension, and air flow rate. It was designed for duct systems in single family residential buildings.
4	Location	LBNL
5	Information Contact	Richard Sextro, LBNL Mark Modera, LBNL
6	Application	Aerosol transport and deposition in straight duct sections
7	Limitations	The model treats indoor aerosol concentrations as being spatially uniform, with two flow regimes. Current model implementation does not account for effects of duct bends, changes in shape, size, etc.
8	Sponsors	Sponsors include California Institute for Energy Efficiency and the U.S. Department of Energy
9	Computer requirement	The model is currently implemented as either a spreadsheet or coded in FORTRAN and will run in a Mac or PC environment or on a workstation.
10	Source-receptor relationship	The model assumes that the aerosol concentration in the duct flow is well-mixed upon entrance.
11	Emission rate	N/A
12	Chemical composition	The model currently treats the aerosols as spheres of uniform composition and assumes that the interaction between the aerosols and the surfaces is physical (and inelastic).
13	Plume behavior	N/A
14	Wind Field	Linear velocities are computed from the duct dimensions and the air flow rate and are compared with the duct Reynolds number to distinguish the flow regime.
15	Dispersion Algorithms	N/A
16	Chemical reactions	N/A
17	Removal processes	As noted, the interaction with surfaces is assumed to take the form of inelastic collisions.
18	Boundary conditions	Dimensions of surfaces; initial conditions include specification of aerosol size and flow.
19	Meteorological requirements	N/A
20	Evaluation	The model has not yet been validated.
21	Output	Tabular outputs (flat ASCII files) can be ported to various graphics programs to provide time series plots, 2-D concentration plots, etc.
22	Genealogy	The model was first formulated to examine efficiency for delivery of aerosoles through a duct system as sealants for duct leaks (where the overall sealing efficiency is a product of the aerosol penetration through the duct and the deposition efficiency in the leaks themselves) (Carrie and Modera 1995).
23	Availability	See 5 above.

1.	Name	**LBNL98**
2.	References	Not yet available
3.	Abstract	Advanced building simulation model which will calculate thermal behavior, intrazonal air flow, ducts and multizone air flow and the generation, transportation and removal of pollutants in complex buildings.
4.	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3058 Berkeley, CA 94720, USA
5.	Contact	Ashok Gadgil Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3058 Berkeley, CA 94720, USA
6.	Applications	Heat transfer, air flow distribution and pollutant transport mechanisms in single-zone and multizone buildings.
7.	Limitations	Not available until late 1998
8.	Sponsors	LBNL Laboratory-Directed R&D Program
9.	Computer Requirements	Parallelized for multiple processor platforms, and UNIX workstations
10.	Conservation Equations	Energy (convection, conduction and radiation heat transfer) and multiple species (generation, transportation and removal)
11.	Fluid Equations	3 dimensional, transient, Reynolds averaged, incompressible, Navier-Stokes with buoyancy production.
12.	Boundary Conditions	Any combination of flux, known property and radiation boundary conditions variable in space and time.
13.	Fluid Properties	Determined from CHEMKIN program
14.	Chemicals	Multiple species tracked separately. Chemical interactions possible through CHEMKIN program.
15.	Origins of Model Approach	Developed by Prof. Harry Dwyer at U.C. Davis (H.A. Dwyer. "Calculation of Droplet Dynamics in High Temperature Environments". Progress in Energy and Combustion Science,. 15, pg. 131, 1989.) based on NASA Ames OVERFLOW code (P.G. Bunning et al, OVERFLOW User's Manual Version 1.7u, 1997)
16.	Solution Method	Finite volume, ADI, Predictor – Corrector solution method, 2nd order in time and space, Pressure projection method used to solve Poisson's equation
17.	Turbulence Models	Two equation turbulence models (k-ε and k-ω) modified for low Reynold's number flow
18.	Radiation Models	Both long wave (thermal infrared) and short wave (visible and solar infrared)
19.	Meshing Method	Overset (Chimera) meshing strategy. Background Cartesian with overlapping generalized curvilinear meshes as needed to capture details of the geometry
20.	Mesh Generators	Public domain hyperbolic (HYPGEN) and elliptic (GRIDGEN) mesh generators as needed.
21.	Output	Output in format for use with TECPLOT

Name	ADPIC	
References	Atmospheric Release Advisory Capability, 1997, "User's Guide to the CG-Mathew/ADPIC Models, Version 5," Lawrence Livermore National Laboratory Report UCRL-MA-103581 Rev.5. Lange, R., 1978, "ADPIC--A Three-Dimensional Particle-in-cell Model for the Dispersal of Atmospheric Pollutants and it Comparison to Regional Tracer Studies," *J. App. Meteor., 17*, pp 320-329. Lange, R., 1989, "Transferability of the Three-Dimensional Air Quality Model Between Two Different Sites in Complex Terrain," *J. Climate and App. Meteor., 28,* pp 665-679. Sherman, C.A., 1978, "A Mass-Consistent Model for Wind Fields Over Complex Terrain," *J. App. Meteor., 17,* pp 312-319. Sullivan, T.S., J.S. Ellis, C.S. Foster, K.T. Foster, R.L. Baskett, J.S. Nasstrom, and W.W. Schalk, III, 1993, "Atmospheric Release Advisory Capability: Real-Time Modeling of Airborne Hazardous Materials," *Bull. Amer. Meteor. Soc. 74,* pp 2343-2361.	
Abstract	The MATHEW model generates a mass conservative three-dimensional gridded mean wind field including terrain effects from available interpolated meteorological data and topography by variational methods. ADPIC is a three-dimensional, numerical diffusion and transport model capable of simulating the time- and space-varying dispersal of atmospheric pollutants under complex conditions. MATHEW/ADPIC are the core models for the DOE Atmospheric Release Advisory Capability (ARAC) Program.	
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551	Source code available from: DOE Energy Science and Technology Center P.O. Box 1020 Oak Ridge, TN 37831
Information Contacts	John S. Nasstrom L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 423-6738 E-mail: jnasstrom@llnl.gov	Connie Foster Phone: (510) 422-1867 E-mail: cfoster@arac.llnl.gov Hoyt Walker Phone: (510) 422-1840 E-mail: hwalker@arac.llnl.gov
Application	Atmospheric transport and diffusion of radioactive and nonreactive toxic chemical releases. MATHEW/ADPIC is the core model used in the Atmospheric Release Advisory Capability which provides DOE HQ, several federal agencies, and numerous DOE and DOD sites with a real-time emergency response modeling service.	
Limitations	MATHEW is a diagnostic model that uses persistence, manual inputs, or gridded wind data for forecasted winds. ADPIC has no reactive chemistry.	
Sponsor	Department of Energy	
Computer Requirements	LLNL runs MATHEW/ADPIC on a VAX/VMS systems (85550, 6610, and 7000 Alphas) It also runs on UNIX workstations. FORTRAN-77 source codes available from ESTSC have been compiled on a variety of systems with more than 3MB of memory.	
Emission Rates	Up to nine releases or species may be specified in a run. Optionally, an unlimited number of nuclides may be specified using the hybrid-particle source term. Emission	

	rates are given in g/s or CI (Becquerel) per second for either gases or particulate matter. Particle size distributions (minimum, mean, maximum and standard geometric deviation off the diameter) must be specified for particulate matter.
Chemical Composition	N/A
Plume Behavior	Release options include the following: • Static source geometry (user specified dimensions) • Plume rise for stack releases using modified Briggs time-dependent buoyant and momentum equations • Explosive cloud rise using Boughton's time-dependent integral plume rise technique • Fires • Reactor accidents involving mixed fission products(an unlimited number of nuclides may be specified using the hybrid-particle source term) • Spills
Wind Field	Three-dimensional vector winds computed by MATHEW
Dispersion Algorithm	Two basic K-theory parameterization dispersion options are available: • Hybrid Eulerian-Lagrangian gradient diffusion • Lagrangian Monte Carlo random displacement diffusion
Chemical Reactions	N/A
Removal Processes	Dry and wet deposition based on deposition velocities and rain rates and gravitational settling base on particle size distribution.
Boundary Conditions	Constant flux in/out flow or reflection at boundary.
Meteorological Requirements	Wind speed and direction at the surface and for at least one vertical profile. Standard deviation of wind direction (s_q), Monin-Obukov length, mixing height, surface roughness (to compute friction velocity), optional temperature profile.
Validation	MATHEW/ADPIC has been extensively evaluated with over a dozen experimental data sets with a wide variety of terrain types, tracer release scenarios, and meteorological conditions. For a summary of validation reports see, Lange(1989) or Sullivan et al. (1993)
Output	Pollutant air concentrations (instantaneous, averaged, or time-integrated) and doses at desired heights and ground-level deposition are written as gridded, two-dimensional arrays. (None of the machine-dependent graphical products are provided with the public-domain ESTSC version.)
Genealogy	MATHEW was initially developed by Christine Sherman and ADPIC by Rolf Lange as the core models for regional-scale dispersion problems in 1975-1978. Since the initial 1979 implementation into the LLNL ARAC emergency response system many improvements have been made including the following: • Controlling the initialization of the wind profiles by either measurements or a parameterized method. • Interpolated three-dimensional wind vectors between meteorological input periods (usually 15 minutes or 1 hour) for each ADPIC time step. • Four-deep nested grids in ADPIC for near-source resolution of concentration and deposition. • Optional K-profile initialization method using sigma theta profile data (validated during DOE Atmospheric Studies in Complex Terrain (ASCOT) program). • Monte Carlo random displacement diffusion option.

Name	**HYPACT**
References	Lyons, W.A. and C.J. Tremback, 1993: A prototype operational mesoscale air dispersion forecasting system using RAMS and HYPACT, Preprints, 86th Annual AWMA Meeting, Denver, CO, 14-18 June 1993.
Abstract	The HYbrid PArticle Concentration Transport model (HYPACT) simulates the motion of atmospheric tracers. The tracer transport is determined from atmospheric flow and turbulence data, typically RAMS model output. HYPACT incorporates a hybrid Lagrangian/Eulerian treatment for tracer transport. The Lagrangian treatment enables the specification of small scale source regions when compared with the grid spacing of the wind model. The hybrid Lagrangian/Eulerian approach represents a tracer by Lagrangian particles near the source region where concentration gradients are large. HYPACT converts particles to Eulerian concentrations at large distances downwind, where the plume is broad and well mixed and grid resolvable.
Location	Mail Stop D-401 Atmospheric and Climate Sciences Group Los Alamos National Laboratory Los Alamos, NM 87545
Information Contacts	General: Craig J. Tremback ASTeR Division of Mission Research Corporation P.O. Box 466 Fort Collins, CO 80522-0466 (970) 282-4400 DOE: James E. Bossart Mail Stop D-401 Los Alamos National Laboratory Los Alamos, NM 87545 (505) 667-6268
Application	Transport and dispersion of non-reactive atmospheric plumes from small scale sources out to hundreds of kilometer distances downwind.
Limitations	Requires a large number of particles be released to adequately define the concentration field. No reactive chemistry or wet deposition.
Sponsor	Primarily Department of Defense
Computer Requirements	Any high-end Unix based work station with FORTRAN and C compilers. Needs sufficient memory and CPU to track large number of particles.
Emission Rates	Releases can be from a specified point, area, or volume anywhere within the domain. Particle releases can be instantaneous, continuous, or over a specified time interval. Any number of particles can be released to represent a known emission rate from a given source. Concentration fields from a known emission are calculated via a particle in cell method.
Chemical Composition	none
Plume Behavior	Non-Gaussian plume described by a large number of tracer particles that are transported by the mean wind and turbulence data.
Wind Field	Three-dimensional, time-dependent winds from a nested grid.
Dispersion Algorithm	Lagrangian first order Markov chain random displacement turbulent diffusion
Chemical Reactions	none
Removal Processes	Dry deposition, gravitational settling, implicit chemical transformation and radiological decay
Boundary Conditions	Reflection or deposition velocity flux boundary condition

Meteorological Requirements	Grid resolved three-dimensional wind field, wind component variances, Lagrangian time scale of wind components
Validation	Ongoing as part of the Emergency Response Dose Assessment System (ERDAS). See Manobiance et al., 1996, *Bulletin of the Amer. Meteor. Soc.* pp 653-672.
Output	Three-dimensional particle positions and air concentrations at any specified time. Post-processing with NCAR graphics includes multicolor plumes from sources over terrain.
Genealogy	RAMS Lagrangian Particle Dispersion Model (LPDM)

Name	**LODI** (Livermore Operational Dispersion Integrator)
References	Leone, J.M., Jr., J.S. Nasstrom, and D.M. Maddix, 1997: A First Look at the New ARAC Dispersion Model, to be presented at the ANS Sixth Topical Meeting on Emergency Preparedness and Response, San Francisco CA, April 22-25, 1997
Abstract	LODI is a three-dimensional, time-dependent, numerical transport and diffusion model capable of simulating the time- and space-varying dispersal of atmospheric pollutants over regions of complex terrain and under complex conditions. This model solves the turbulent, advection-diffusion equation via a Lagrangian particle, Monte-Carlo method. Within a simulation, particles representing the pollutant are moved through the domain using a random displacement method to model the turbulent diffusion and a Runge-Kutta method to model the advection.
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551
Information Contacts	John M. Leone, Jr. L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 422-6449 E-mail: jleone@llnl.gov
Application	Atmospheric transport and diffusion of radioactive and nonreactive toxic chemical releases. This model is designed to be used in an emergency response mode.
Limitations	No reactive chemistry. Use of advection-diffusion random displacement method limits accuracy for times less than the Lagrangian time-scale.
Sponsor	Department of Energy
Computer Requirements	Model requires only a computer with a valid Fortran-90 compiler. However, the size of memory will determine the number of particles that can be released during any simulation. LODI has been run on Sun Sparc II, SGI Indy and Indigo 2, desktop workstations, on DEC alpha servers, and Cray C-90.
Emission Rates	Releases may be from either static or time dependent source geometries. Either instantaneous or time dependent continuous releases are modeled. An unlimited (subject to computer memory) number of species may be specified. Emission rates are given in g/s or Ci/s for either gases or particulate matter. Particle size distributions must be specified for particulate matter.
Chemical Composition	N/A
Plume Behavior	Non-Gaussian plume described by a large number of marker particles which move through the domain.
Wind Field	Three-dimensional, time-dependent gridded winds (can be on nested grids) are model input.
Dispersion Algorithm	Lagrangian Monte-Carlo random displacement turbulent diffusion
Chemical Reactions	N/A
Removal Processes	Dry and wet deposition and gravitational settling.

Boundary Conditions	Reflection at boundary or deposition velocity flux boundary condition
Meteorological Requirements	Gridded (u, v, w) wind fields, turbulence parameters depending upon which option chosen e.g. ustar, boundary layer depth, Obukov length, Lagrangian time scale
Validation	Just beginning - code under development.
Output	Pollutant air concentrations (instantaneous or time-integrated) at desired heights and ground-level deposition are written as gridded, two-dimensional arrays in netCDF files. Three dimensional air concentrations (instantaneous or time-integrated) may also be written to netCDF files. Visualization is done via a post-processor.
Genealogy	This a new model currently under development.
Additional Remarks	Requires FORTRAN-90 compiler and netCDF file handling library.

Name	**RAPTAD**
References	Williams and Yamada, 1990: A microcomputer-based forecasting model: potential applications for emergency response plans and air quality studies, *JAWMA*, *40,* pp 1266-1274. Williams, Brown, Cruz, Sosa, and Streit, 1995: Development and testing of meteorology and dispersion models for Mexico City, *At. Env., 29*, pp 2929-2960.
Abstract	RAPTAD is a three-dimensional, time-dependent, numerical transport and diffusion model. It uses a computationally efficient combined random-walk/puff approach which allows it to release a smaller number of puffs (particles) than a traditional random-walk method and still obtain smooth, continuous concentration profiles.
Location	Energy & Environmental Analysis Group Los Alamos National Laboratory Los Alamos, NM 87545
Information Contacts	Mike Williams or Michael Brown (505) 667-1788
Application	Complex dispersion in coastal, mountainous, and urban areas. Models point, line, or area sources.
Limitations	Must be able to specify Lagrangian time-scale. No dense gas capability
Sponsor	Department of Energy
Computer Requirements	Fortran77 versions of the model exist for Unix and IBM platforms.
Emission Rates	Either instantaneous or continuous releases of neutral or buoyant pollutants are modeled for both ground-level and elevated sources.
Chemical Composition	N/A
Plume Behavior	Lagrangian, random-walk puff. Puffs are released one after another. They grow with time due to entrainment and travel on a random-walk using an externally supplied mean wind field and an internally computed Monte-Carlo turbulent wind.
Wind Field	Three-dimensional, time-dependent gridded winds are model input.
Dispersion Algorithm	Lagrangian Monte-Carlo random-walk and puff growth using random-force theory.
Chemical Reactions	Version called RAPBOX has carbon-bond chemistry.
Removal Processes	Deposition
Boundary Conditions	Reflection at ground. Reflection or partial penetration at boundary layer top according to stratification and turbulence intensity.
Meteorological Requirements	Gridded wind, temperature, and turbulent kinetic energy fields; usually from Mesoscale model HOTMAC, but data from other models accepted.
Validation	Mexico City Air Quality Research Initiative - reported in Williams et al., 1995 (see above.) U.S. Army, Toole Depot Study, reported in Williams and Yamada, 1990 (see above.) Cross Appalachian Tracer Experiment - Kao and Yamada, 1988: Use of the CAPTEX data set for evaluations of a long-range transport numerical model with a 4D data assimilation technique, *MWR, 116*, p 293. DOE ASCOT - Brush Creek - Yamada and Bunker, 1988: Development of a nested

	Grid 2nd Moment Turbulence Closure Model and Application to the 1982 ASCOT Brush Creek Data Simulation, *JAM, 27*, p 562. DOE ASCOT - Geysers -Yamada, 1985: Numerical Simulation of the Night 2 Data of the 1980 ASCOT experiments in the California Geysers Area, *Arch. Met. Geoph. Biocl. Ser. A., 34*, p 223.
Output	Pollutant air concentrations in file formats for NCAR graphics, Spyglass 2D and 3D software, AVS, and Deltagraph software.
Genealogy	
Additional Remarks	

Name	**SLAB**
References	DOC OFCM Modeling Resources.
Abstract	The SLAB model, developed by Lawrence Livermore National Laboratory, was enhanced by LLNL under support of AFESC. The model treats denser-than-air releases by solving the one-dimensional equations of momentum, conservation of mass, species, and energy and the equation of state. SLAB handles release scenarios including ground-level and elevated jets, liquid pool evaporation, and instantaneous volume sources. The model accounts for user-selected averaging time effects.
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551
Information Contacts	Don Ermak L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 423-0146 E-mail: ermak1@llnl.gov
Application	Denser-than-air dispersion
Limitations	Plume model with straight line wind field.
Sponsor	
Computer Requirements	IBM PC-compatible in MS_DOS operating environment; FORTRAN-77 language.
Emission Rates	Point, area, instantaneous, and continuous
Chemical Composition	Ground-level/elevated jets, liquid pools of hazardous chemicals.
Plume Behavior	Gaussian plume
Wind Field	Straight line
Dispersion Algorithm	K-diffusivity, heavier-than-air dispersion
Chemical Reactions	None
Removal Processes	None
Boundary Conditions	
Meteorological Requirements	Temperature and point winds
Validation	Approved by EPA as a hazardous chemical dispersion model. Recognized in API hazardous chemical model evaluation.
Output	Concentrations
Genealogy	
Additional Remarks	Aerosol two-phase release